

# Many-body fits of phase-equivalent effective interactions

Calvin W. Johnson

*Department of Physics, San Diego State University,  
5500 Campanile Drive, San Diego, CA 92182-1233*

In many-body theory it is often useful to renormalize short-distance, high-momentum components of an interaction via unitary transformations. Such transformations preserve the on-shell physical observables of the two-body system (mostly phase-shifts, hence unitarily-connected effective interactions are often called phase-equivalent), while modifying off-shell T-matrix elements influential in many-body systems. In this paper I lay out a general and systematic approach for controlling the off-shell behavior of an effective interaction, which can be adjusted to many-body properties, and present an application to trapped fermions at the unitary limit.

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The force between two particles has to be determined empirically, but some matrix elements are easier to determine than others. For an isolated two-body system one can measure elastic phase shifts and bound state eigenvalues, but not off-shell (inelastic) matrix elements (specifically, the elements of the T-matrix). Such matrix elements show up when the two-body system is not isolated, i.e., embedded in a many-body system, but disentangling the off-shell two-body matrix elements from many-body data is not possible.

Following modern trends in effective interaction theory [1–5], I will argue that one can flip the ambiguity of off-shell matrix elements into an advantage. This paper illustrates a general method to find the unitary transformation that preserves two-body observables while simultaneously providing the best fit to many-body data.

For example, despite much effort we do not have a unique prescription for the force between nucleons. Nonetheless high-precision data on two-nucleon systems [6] strongly constrain any description, leading to a variety of competing interactions [7–10] which all, by construction, have indistinguishable on-shell T-matrix elements; these are called phase-shift equivalent potentials. The off-shell T-matrix elements, which *do* differ, can only be compared through many-body observables, including binding energies and excitation spectra.

In a parallel vein, consider configuration-interaction (CI) many-body calculations, which have several advantages but are vulnerable to strong short-range, high-momentum components of the interaction, because practical considerations require truncation, indicated by a projection operator  $\hat{P}$ . The problem is the eigenvalues of  $\hat{P}\hat{H}\hat{P}$  are not the same as the eigenvalues of  $\hat{H}$  in an infinite or even very large space, and converge slowly with increasing dimension of  $\hat{P}$ , a particularly severe problem for CI calculations. Therefore one turns to effective interactions, generated using a unitary transformation

$$\hat{H}_{\text{eff}} = \hat{U}^\dagger \hat{H} \hat{U}. \quad (1)$$

The hope is that the eigenvalues of  $\hat{P}\hat{H}_{\text{eff}}\hat{P}$  in the truncated space converge to those of  $\hat{H}$  in an infinite space. One common strategy is the so-called ‘cluster approximation’: forcing the eigenvalues in the truncated space

to agree with the ‘exact’ values of the original space, but only for two- (or on occasion three-) particle systems, and then apply to many-body systems.

Modern, rigorous effective interaction methods explicitly or implicitly apply a unitary transform that leave the on-shell behavior unchanged but which dial away the troublesome high-momentum part of the interaction. These methods, which include but are not limited to Okubo-Lee-Suzuki (OLS) [1], the unitary correlation operator method (UCOM) [2], the similarity renormalization group (SRG) [3], and Alhassid-Bertsch-Fang (ABF) [4], generate a portfolio of new ‘phase-equivalent’ interactions with the same on-shell T-matrices but different off-shell matrix elements.

The two-body cluster approximation is complicated by the fact that three-body forces naturally arise out of effective field theory [10, 11]. In practice, however, three-body forces make for computational difficulties. Thus several authors have sought to *minimize* three-body forces by exploiting the interplay between three-body forces and off-shell matrix elements [2, 12, 13].

This paper combines several of these ideas. Borrowing from phenomenological fitting of interactions [14, 15], I show how one can choose a general unitary transformation to generate a phase-equivalent potential which is a “best fit” to many-body data.

To illustrate, I take on a specific challenge: spin-1/2 fermions at the unitary limit, the so-called “Bertsch problem,” in the context of an external harmonic trap [16, 17]. The interaction is zero range and has infinite scattering length, similar to the short-range, large scattering length nuclear force. The Hamiltonian is

$$\hat{H} = \sum_i -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m \Omega^2 r_i^2 - V_0 \sum_{i < j} \delta^{(0)}(\vec{r}_i - \vec{r}_j). \quad (2)$$

The ground state energy for the 3-body case is known analytically [18], and for  $N \geq 4$  I take as ‘exact’ the results from correlated Gaussian and fixed-node diffusion Monte Carlo calculations [17] (with quoted statistical and systematic errors of only a few percent, which I leave out). Table I lists the energies adopted in this study. For purposes of comparison I group the energies into two

sets: Set I includes the ground states and selected excited states for  $N = 3, 4$ , while Set II is comprised of the ground state energies for  $N = 3-10$ .

TABLE I: Adopted energy levels [17, 18] in units of  $\hbar\Omega$  of the trapping potential and assignment to comparison sets.

$N$	$L^\pi; S$	energy	Set
3	$1^-; \frac{1}{2}$	4.27	I,II
	$0^+; \frac{1}{2}$	4.66	I
4	$0^+; 0$	5.05	I,II
	$2^+; 0$	5.91	I
	$1^+; 1$	6.58	I
5	$1^-; \frac{1}{2}$	7.53	II
6	$0^+; 0$	8.48	II
7	$1^+; \frac{1}{2}$	11.36	II
8	$0^+; 0$	12.58	II
9	$0^+; \frac{1}{2}$	15.69	II
10	$0^+; 0$	16.80	II

The Hamiltonian (2) can be separated into the center of mass plus the relative Hamiltonian:

$$\hat{H}_{\text{rel}} = -\frac{\hbar^2}{2\mu}\nabla_r^2 + \frac{1}{2}\mu\Omega^2 r^2 - V_0\delta(r) \quad (3)$$

where  $\vec{r} = \vec{r}_1 - \vec{r}_2$  is the relative coordinate and  $\mu = m/2$  the reduced mass. For application to configuration interaction (CI) calculations, one computes the matrix elements of  $\hat{H}_{\text{rel}}$  in a harmonic oscillator basis,  $\langle n'l|\hat{H}_{\text{rel}}|nl\rangle$  (which are only nontrivial for the relative  $s$ -wave or  $l = 0$ ), and then transform to the lab frame two-body matrix elements via Brody-Moshinsky brackets [19].

I truncated the relative space to  $n_{\text{cutoff}} = 5$ , which means for  $\langle n'l|\hat{H}_{\text{rel}}|nl\rangle$  I use  $n, n' = 1, \dots, 5$ ; this corresponds to including up  $8\hbar\Omega$  in excitation energy in the relative space. (Calculations with different  $n_{\text{cutoff}}$  had similar results.) For the lab frame, also using a harmonic oscillator basis, I truncated the single-particle space to four major shells, that is,  $0s$ ,  $0p$ ,  $1s0d$ , and  $1p0f$ .

The  $\delta$ -interaction must be regularized to fix the scattering length; for CI calculations in an oscillator basis, the interaction strength  $V_0$  depends on  $n_{\text{cutoff}}$ , the number of  $s$ -wave basis states used. For the ‘bare’ interaction, fixing the scattering length is equivalent to fixing the ground state energy of the relative two-body state [4, 5, 20]; due to truncation, the excitation energies differ from the infinite space values. Alternately, I also used, in the  $n_{\text{cutoff}} = 5$  space, the ABF interaction, which fixes all five eigenenergies of  $\hat{H}_{\text{rel}}$  in the truncated space to the correct (infinite space) values.

Going to three or more particles immediately illustrates some of the headaches of effective interactions, as can be seen in Table II. Consider the rms error between calculated and target (experimental) energies,

$$[\sum_{\alpha} (E_{\alpha}(\vec{c}) - E_{\alpha}^0)^2]^{1/2}. \quad (4)$$

For ‘bare’ interactions, the rms error on Set II (ground state energies, in units of  $\hbar\Omega$  of the trapping potential, for  $A=3-10$ ) is 1.16, while for ABF it is 2.32. That is, forcing the effective interaction to have the correct eigenvalues for the two-body system can lead to larger errors in the many-body system. (This comparison, oversimplifies the story; please read the original [4].)

TABLE II: Root-mean-square error between adopted exact energies (Table I) and calculated CI energies. ‘Starting  $\hat{H}_{\text{rel}}$ ’ refers to using either the ‘bare’ or ABF regularized interaction (see text). ‘Generators’ refer to the set of operators used in the unitary transformation to minimize the rms error: ‘none’ means no transformation was performed, ‘all’ means all ten generators were used, and  $d/dr$  denotes using only the single generator  $d/dr$  in the relative space. Units are  $\hbar\Omega$  of trapping potential. The unitary transformations were fit to either Set I or II; ‘I  $\rightarrow$  II’ refers to fitting to Set I, but computing the rms error on Set II.

Starting $\hat{H}_{\text{rel}}$	Fit Set	Generators		
		none	$d/dr$	all
bare	I	0.62	0.19	0.10
bare	I $\rightarrow$ II	(1.16)	0.55	0.32
bare	II	1.16	0.31	0.28
ABF	I	1.06	0.11	0.06
ABF	I $\rightarrow$ II	(2.32)	0.58	0.37
ABF	II	2.32	0.26	0.25

The apparent paradox of a bare interaction doing better than a renormalized one can be understood by writing  $\hat{U} = \exp(\hat{A})$ , where  $\hat{A}$  is an anti-Hermitian two-body operator. Then  $\hat{U}$  induces many-body terms in  $\hat{H}_{\text{eff}}$  cutoff by the two-body cluster approximation.

Previous authors made specific implicit choices in the form of their off-shell behavior to minimize the effect of three-body interactions. The strength of the correlation operator in UCOM [2], which shifts nucleons away from each other, is fit to minimize the error in the  $A = 3$  and 4 ground state energies. The inside-nonlocal, outside-Yukawa (INOY) potential [12] is adjusted to both two-body data plus the triton binding energy, while the  $J$ -matrix inverse scattering potential (JISP16) is fit to two-body data plus binding energies up to  $^{16}\text{O}$  [13].

I propose a general method to choose the ‘best’ unitary transformation. Expand  $\hat{A}$  in a set of generators

$$\hat{A} = \sum c_i \hat{A}_i. \quad (5)$$

The dependence of the calculated many-body eigenenergies  $\{E_{\alpha}(\vec{c})\}$  on the  $c_i$  can be expanded to first order

$$E_{\alpha}(\vec{c}) \approx E_{\alpha}(0) + \sum_i \frac{\partial E_{\alpha}}{\partial c_i} c_i \quad (6)$$

The required derivatives can be found via the Hellman-Feynman theorem [21]:

$$\frac{\partial E_{\alpha}}{\partial c_i} = \langle \alpha | [\hat{H}, \hat{A}_i] | \alpha \rangle \quad (7)$$

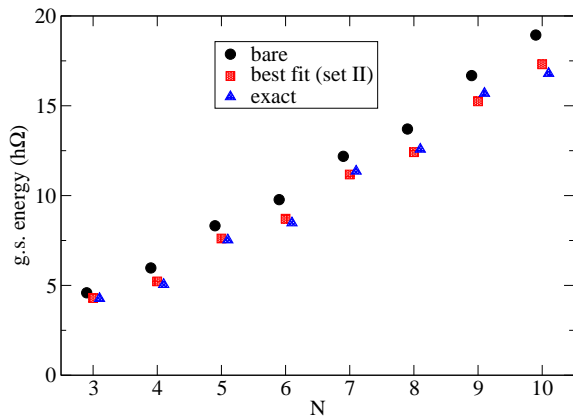


FIG. 1: (Color online) Comparison of ground state energy for  $N$  particles in a harmonic trap, interacting via a contact interaction: (black) circles are “bare” results (fixed in relative frame at  $n_{\text{cutoff}} = 5$ ), (red) squares are the best fit of all generators of a unitary transformation, and (blue) triangles are the exact results. All energies in units of  $\hbar\Omega$  of the trapping potential. Slight horizontal offshifts were introduced to aid visibility.

Now consider a target set of (experimental) many-body energies  $\{E_\alpha^0\}$ . By minimizing the root-mean-square difference (4) between calculated and target (experimental) energies, one obtains

$$\sum_j \left( \sum_\alpha \frac{\partial E_\alpha}{\partial c_i} \frac{\partial E_\alpha}{\partial c_j} \right) c_j \approx \sum_\alpha (E_\alpha^0 - E_\alpha) \frac{\partial E_\alpha}{\partial c_i} \quad (8)$$

which can be solved for the  $c_i$ . Because Eq. (8) is only a linear approximation, one may need to iterate to converge on a best solution. This methodology is very similar to that used to fit two-body matrix elements to low energy nuclear spectra [14, 15], except that in those cases one directly fits Hamiltonian matrix elements in the lab frame, and here I fit the coefficients of generators of a unitary transformation (and in my application below I work in the relative frame).

(As an important technical point, the matrix  $M_{ij} = \sum_\alpha \frac{\partial E_\alpha}{\partial c_i} \frac{\partial E_\alpha}{\partial c_j}$  is in general nearly singular, so one uses singular value decomposition [22, 23] to find the dominant modes. Here singular value decomposition is nothing more than using a spectral (eigenvalue) representation of  $M_{ij}$  and keeping only nonsingular terms.)

This methodology is flexible and general. One can use as many or as few generators as desired or thought physically relevant, and can constrain to a best fit using an arbitrary choice of many-body energies.

I applied this prescription to my example system. As described above, in the relative space  $\langle n', l = 0 | \hat{H}_{\text{rel}} | n, l = 0 \rangle$  with  $n_{\text{cutoff}} = 5$  is a  $5 \times 5$  real symmetric matrix (using either the ‘bare’ or ABF matrix elements). I then introduced a general real orthogonal transformation as in Eq. (1), where  $\hat{U}$  also is a  $5 \times 5$  matrix, with 10 possible antisymmetric generators  $\hat{A}_i$ . (I only performed

the transformation in the relative  $s$  channel. In principle an effective interaction could generate nontrivial matrix elements in other channels. I leave this to future investigations.) I then fit the parameters  $c_i$  in Eq. (5) by minimizing the rms error on either Set I or Set II. The results are shown in Table II (the energies are all in units of  $\hbar\Omega$  of the trapping potential) and illustrated in Figure 1. There is a dramatic reduction in the rms error.

The best fit parameters for Sets I and II differed, of course. I also considered the error in extrapolation, by fitting to Set I but calculating the rms error on the larger Set II; found in Table II in the rows marked ‘I→II,’ the error in extrapolation is at worst fifty percent larger than the best fit to Set II. (The first number in these rows, in parentheses, is the original rms error, as there is no fit.)

Interestingly, although ABF starts with a larger rms error, it yields fits with smaller errors.

By insisting that the on-shell two-body matrix elements (relative-space eigenvalues) remain invariant, and keeping only the  $s$ -wave relative channel, the above is the best fit that one can obtain. The remaining residual error is due to induced three-body forces that cannot be fully replicated using a two-body force [24].

The SVD of  $M_{ij}$  was always dominated by one or two eigenvalues and thus one or two generators. In addition, one would appreciate simple physical insights into the unitary transformation. I therefore tried the manifestly antisymmetric generator  $d/dr$  (where  $r$  here is the relative coordinate), because of simplicity but also because of similarity to UCOM [2]. Table II shows this single generator significantly reduces the rms error.

The minimization will be model-space dependent, but one can see this as either a weakness or a strength. Most many modern interactions already have an intrinsic cutoff dependence. Here I have given how to best “tune” an effective interaction to a model space. One can also choose key energy levels to fit to, not only ground state energies but excited states that contain important physics such as spin-orbit splitting. Also, critically, it will be important to constrain the unitary transformation to other observables such as the rms radius. Given that only a few degrees of freedom were used to minimize the energies, this is not impossible and is under investigation.

To summarize, I have discussed general unitary transformations which produce effective interactions, and have shown how one can use many-body data to improve the interaction while preserving eigenvalues in the relative space (on-shell T-matrix elements). This methodology is a generalization of modern effective interaction theory and of previous specific attempts to reduce the need for three-body interactions. With a simply defined yet numerically challenging case of trapped fermions at the unitary limit, I demonstrated improvement in ground state energies.

One of the claims of current methods is they provide reliable error estimates for predictions. While I have not addressed this important issue, one should see that the

error estimates are dependent on the choice of unitary transformation, an issue that has not yet been addressed in a deep way. At least I hope to provoke a closer investigation of competing effective interaction methodologies (and their claimed error estimates): OLS, SRG, UCOM, and other specific choices.

Extending this work to nuclei and to the inclusion of

observables is under way.

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